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Charged Particle Transport in FLAG

Edward Norris



Managed by Triad National Security, LLC for the U.S. Department of Energy's NNSA

Outline

- Motivation
- Charged particle transport theory
- Implementation
- Usage
- Test Problems
- Future work



Motivation

Motivation

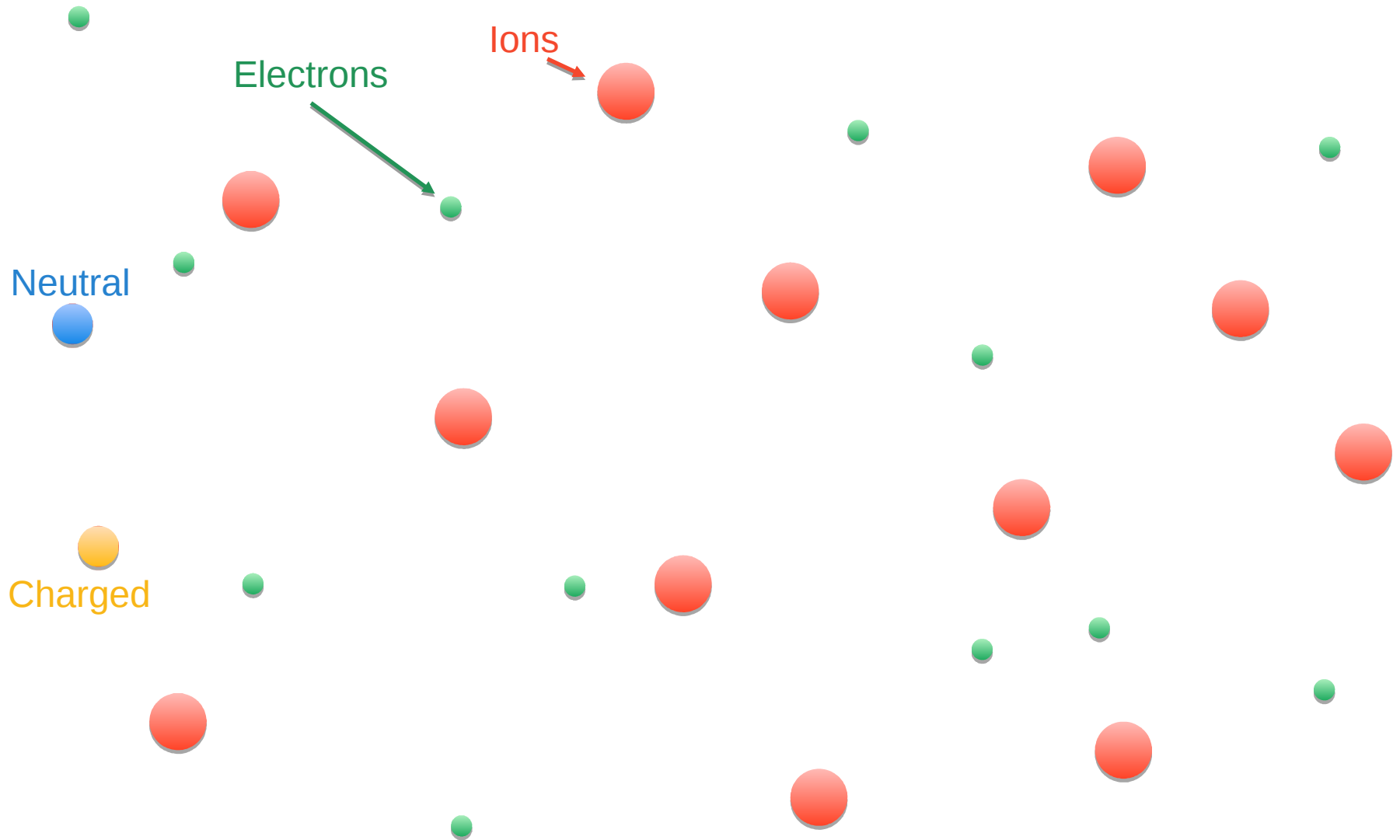
- Currently, all energy deposition is local
 - All energetic particles born in a zone deposit 100% of their energy in that zone
- Charged particles deposit energy over 10s to 100s of microns.
- As advanced hardware and ICF capsule design drives zone sizes below this threshold, local deposition is no longer a good approximation.
- Motivates implementation of a Monte Carlo charged particle transport package

Charged Particle Transport Theory

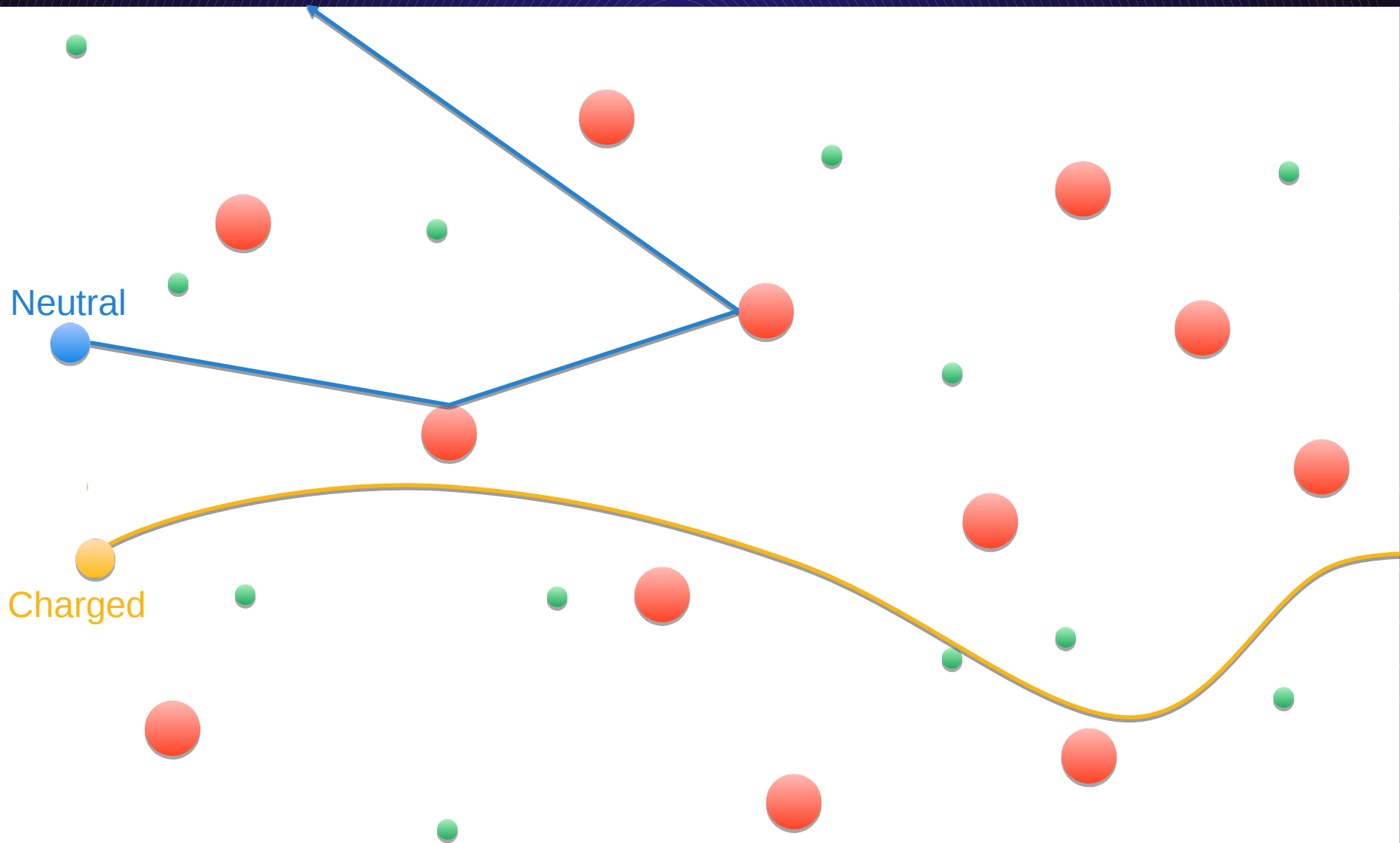
Theory

- All equations implemented must use SI units!

Theory

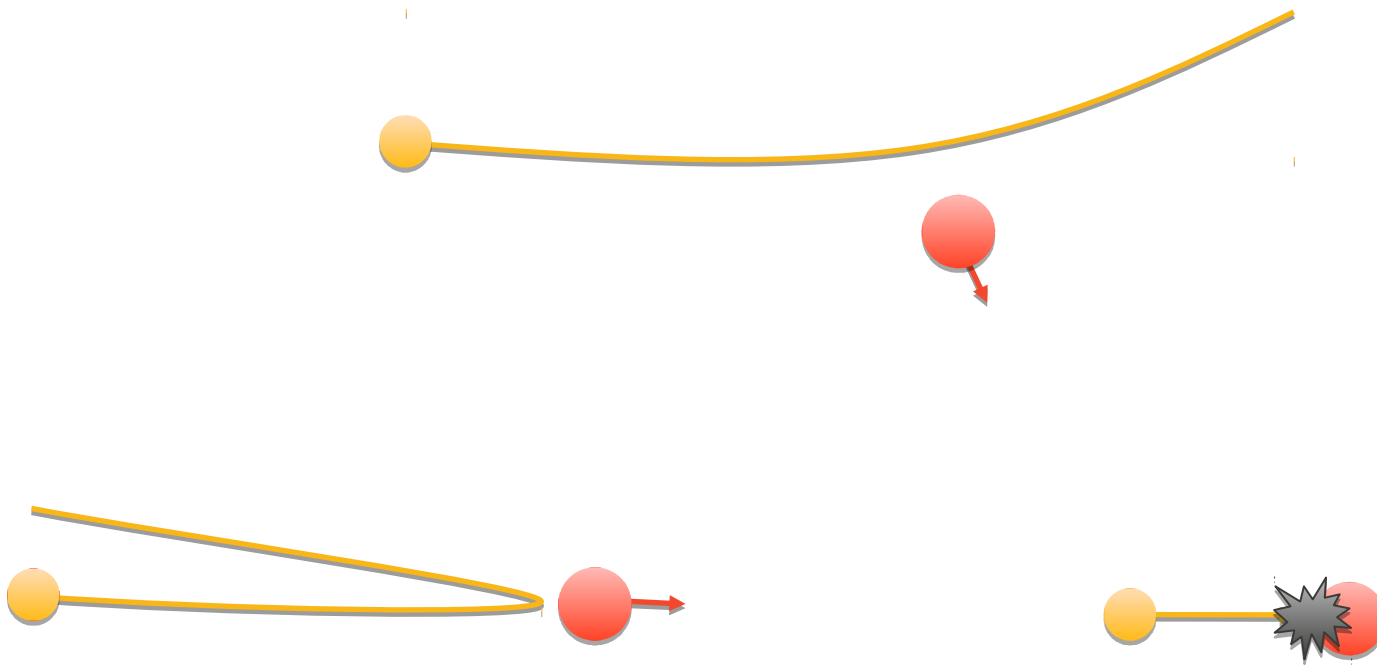


Theory



Theory

- As particles move around, they undergo two types of interactions:
 - Small angle scatter
 - Catastrophic interactions

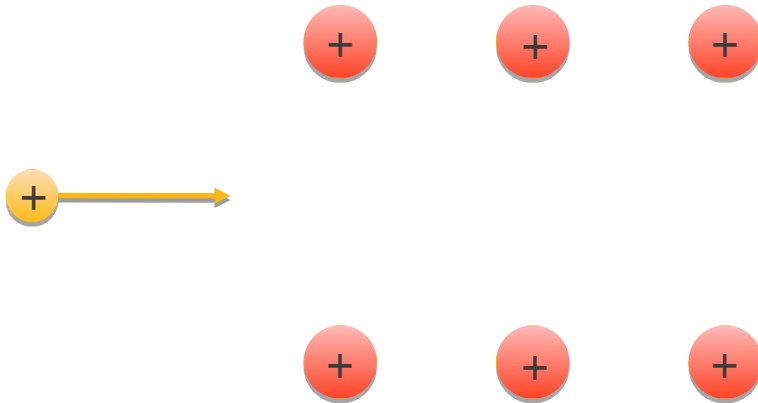


Theory

- Small angle scatter is dominated by Coulombic interactions
 - Each small path length can be treated as a line
 - Advance the particle, compute the energy loss, repeat
 - Assume that on average, scatters cancel out and the particle travels in a straight line
- Catastrophic interactions result in the particle being killed off
 - Local energy deposition wherever the particle is
 - **Not modeled yet**
- Currently, particles travel in a straight line and deposit energy as they travel.

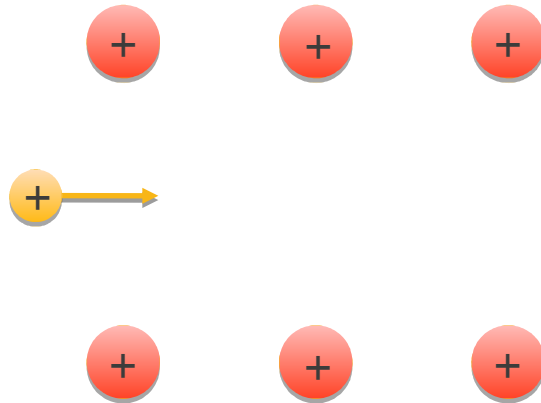
Theory

- Consider a charged particle flying through a “tunnel” of ions



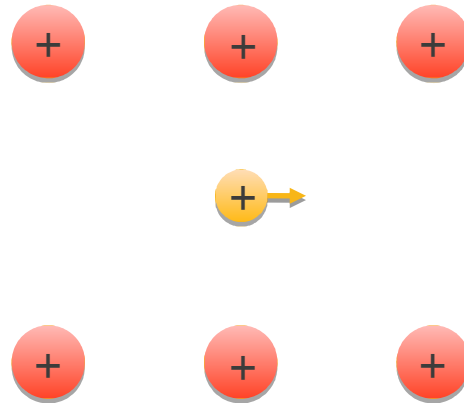
Theory

- The particle slows as it is repelled



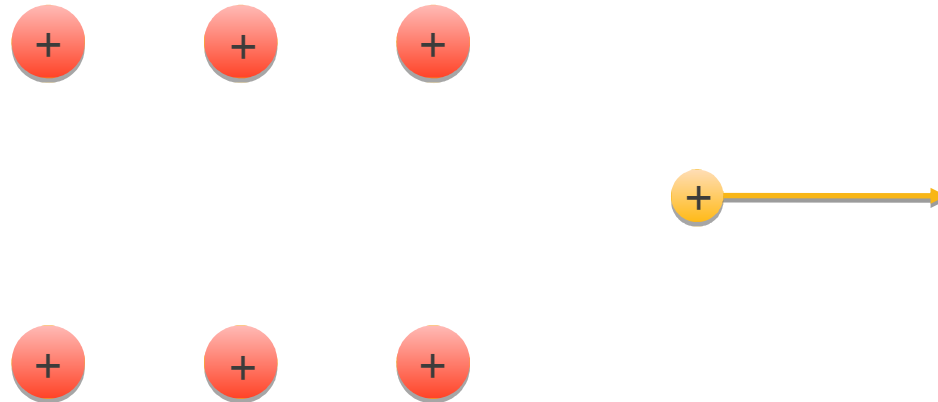
Theory

- Halfway, there is no net force on the particle



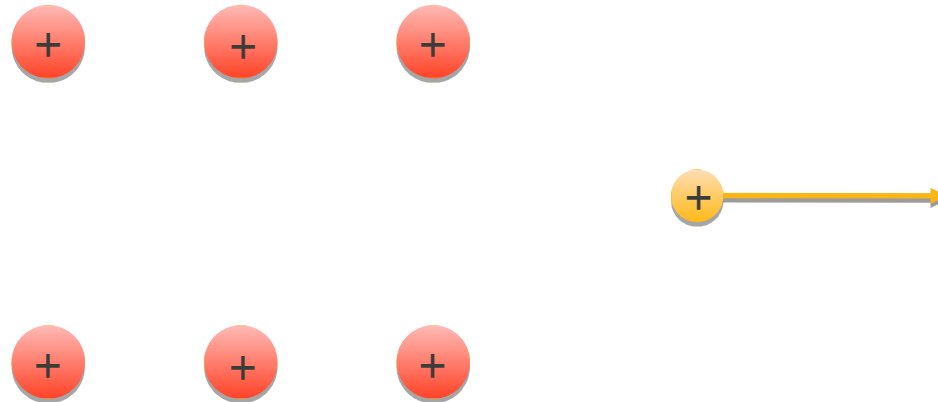
Theory

- On the way out, the particle is repelled and accelerates. It gains the same amount of energy it lost going in.



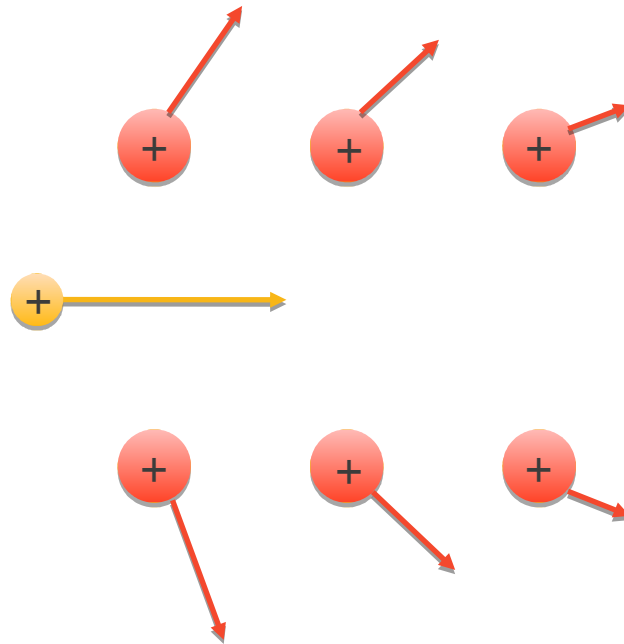
Theory

- How can charged particle interactions result in an energy transfer?



Theory

- As the particle approaches, it accelerates the ions and they move further away



Theory

- And the particle is not accelerated while leaving as much as it was decelerated entering



The energy imparted to the ions is equal to the loss in energy of the charged particle due to the displacement of the ions



Timescale is very important!



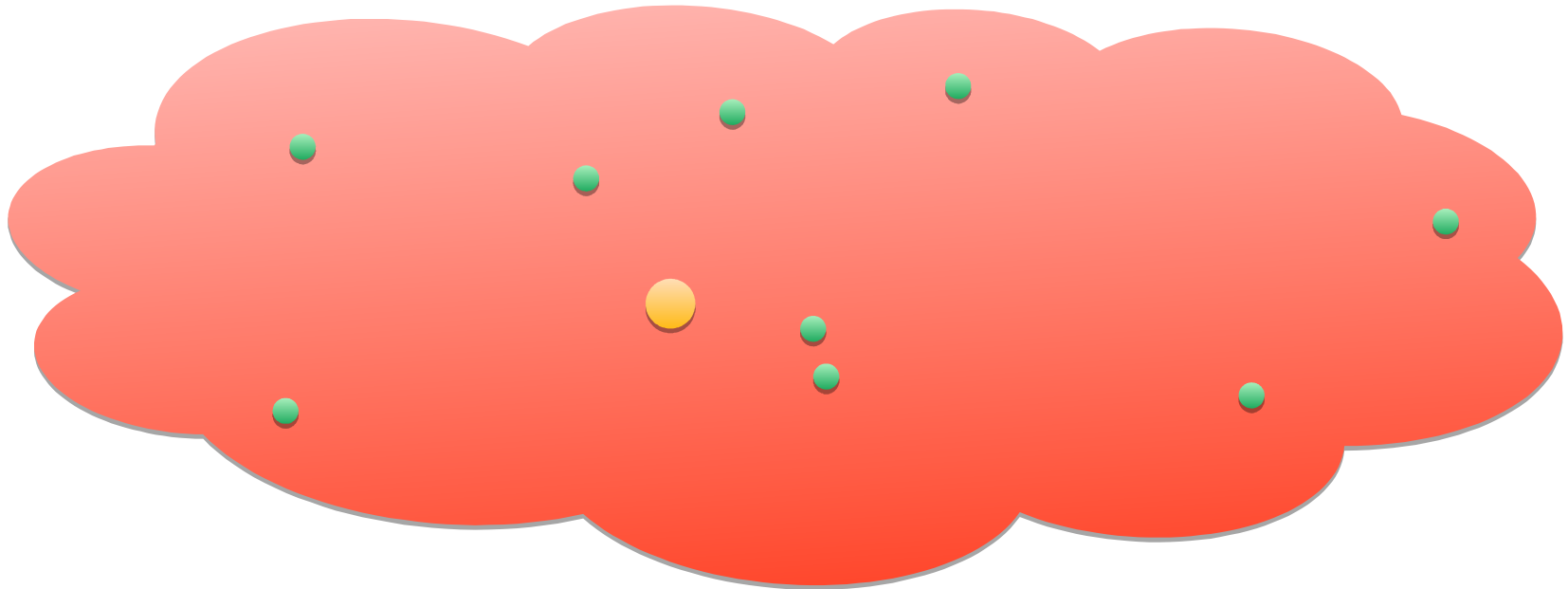
Theory

5 keV, D-T plasma

3.5 MeV α

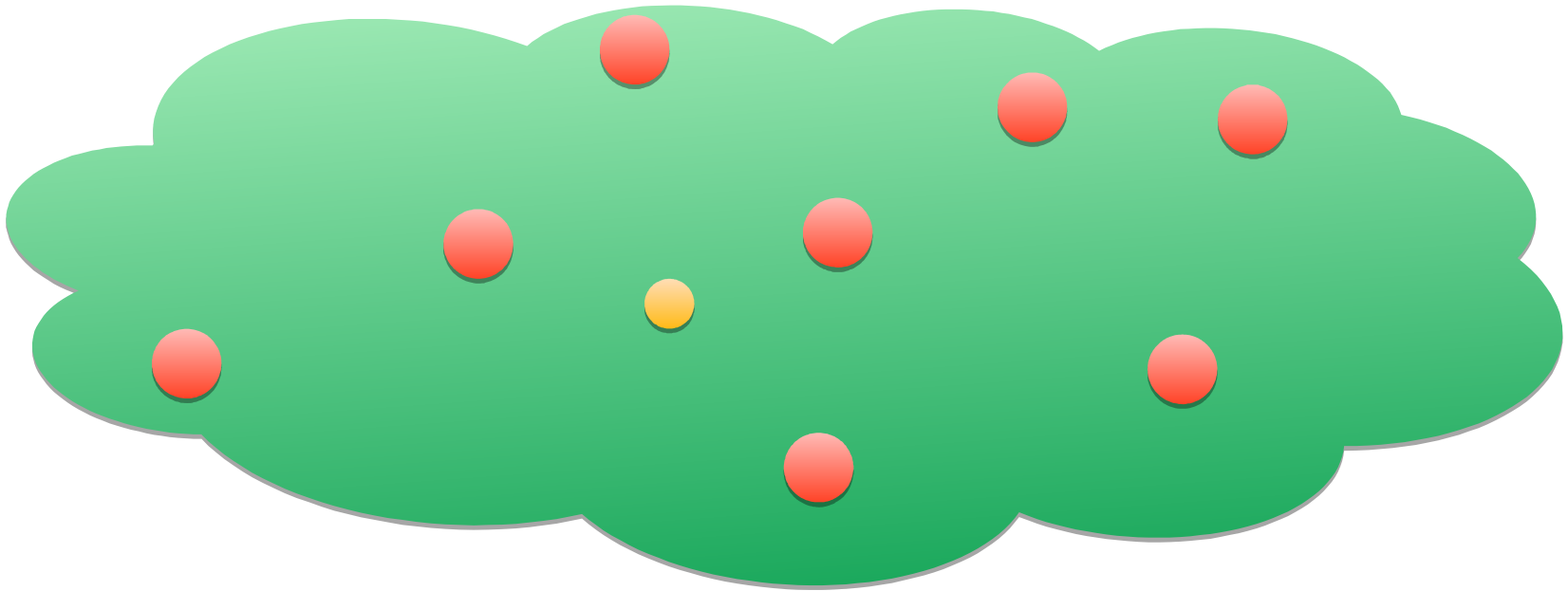
Theory

- DT Ions ($m = \sim 2.5$ amu, $E = 5$ keV)
 - Speed: 62.1 cm/ μ s
- DT Electrons ($m = 0.00055$ amu, $E = 5$ keV)
 - Speed: 4190 cm/ μ s
- Charged Particle ($m = 4.0$ amu, $E = 3.5$ MeV)
 - Speed: 1300 cm/ μ s



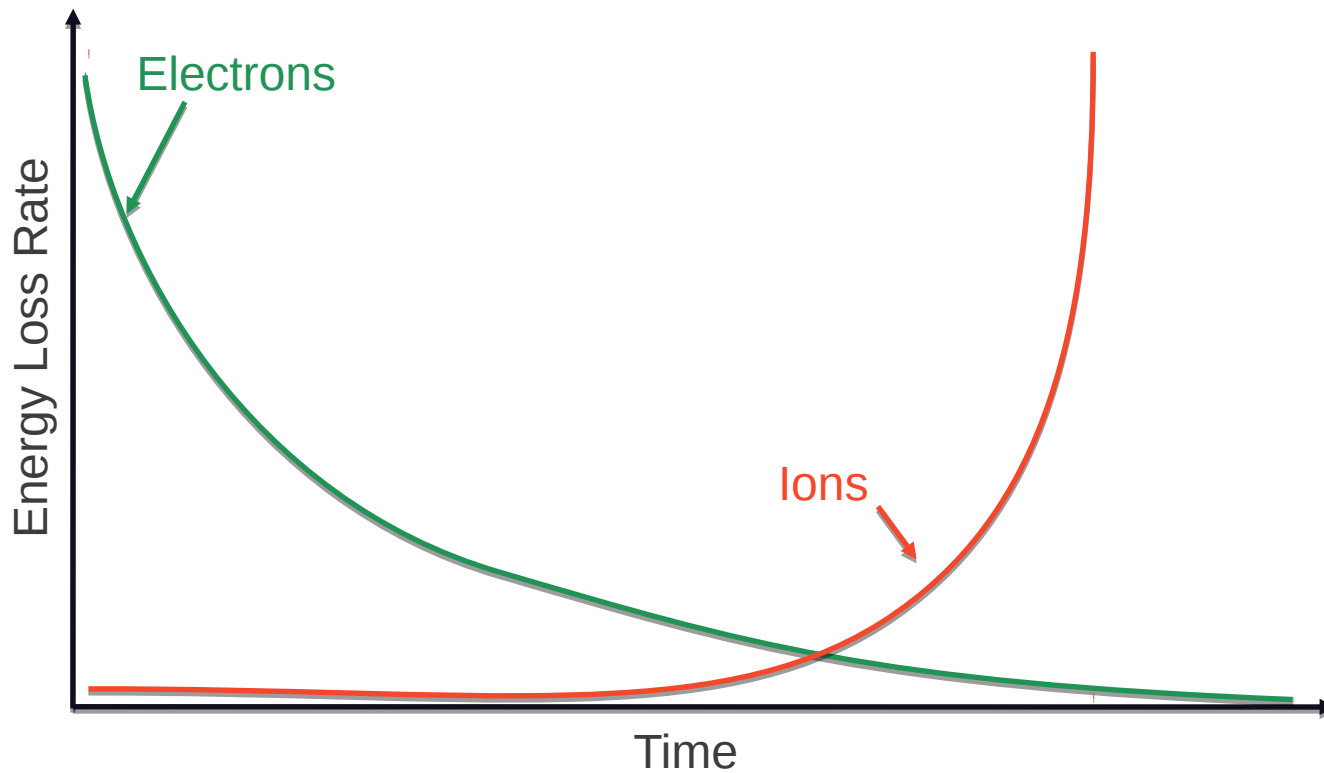
Theory

- As the charged particle interacts with electrons, it loses energy
- Eventually, the particle is going at approximately the same speed as the ions and much slower than the electrons



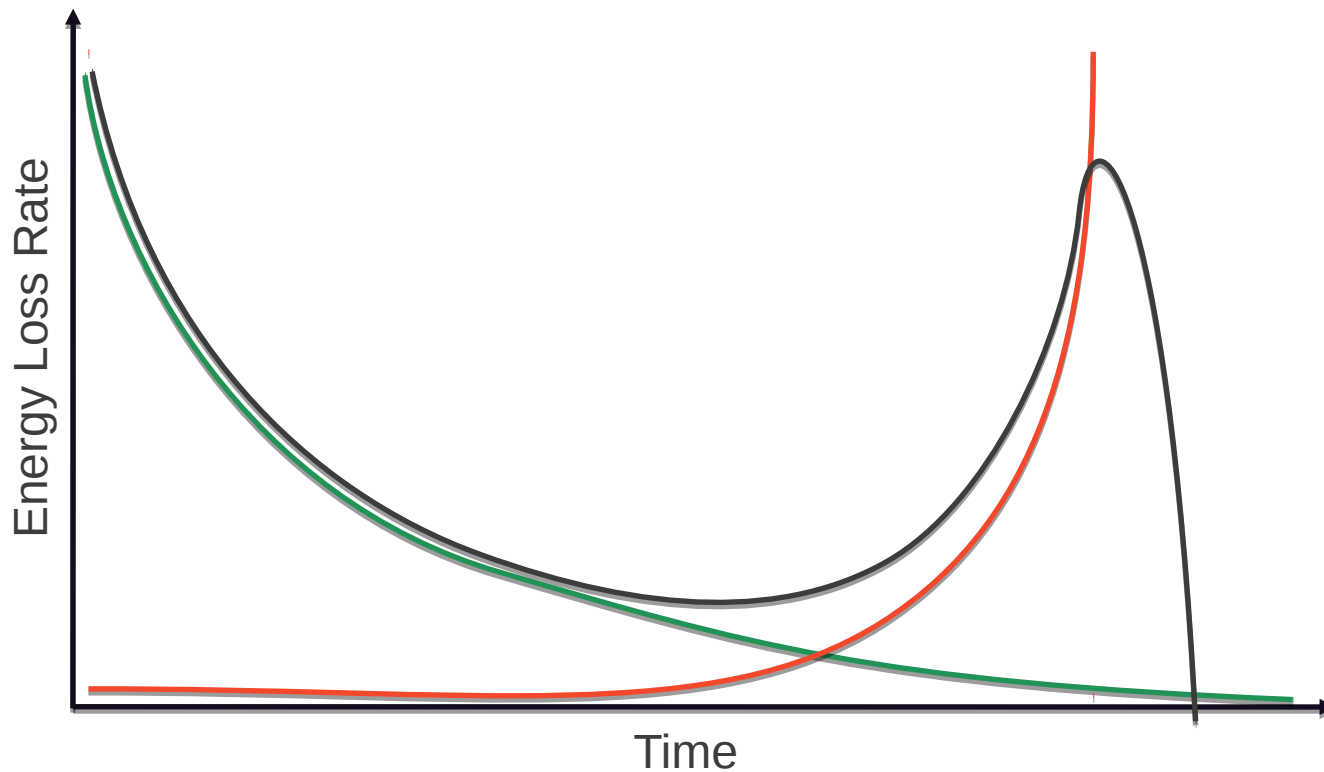
Theory

- Dominant interaction changes over time



Theory

- At some point, the particles drop to the same temperature as the background plasma and stop losing energy altogether



Theory

- Four models

Void

No physics – particles travel in straight line and do not slow down

Simple

Analytic

dE/dx Data

Based on electrons only. Has an ion correction that can be turned on

Theory

- Four models

Void

Simple

Analytic

dE/dx Data

Based on Plasma Formulary
equations



Multiple datatable correlations
available

Implementation

Implementation

DoFlagDriver(kdd)

```
...  
call MixDriver(mesh)  
call SBroad('PrePhysCycle', mesh, dtg)  
call SBroad('ChargedPtcPhys', mesh, dtg)  
ncount = 0  
call SBroad('CalcEIRSrc', mesh, ncount)  
if(ncount.gt.0)then  
...  
enddo
```

ChargedPtcPhys(this, dtg)

```
call SBroad('SpawnCharged', this, dtg)  
call SBroad('MoveCharged', this, dtg)
```

ChargedPtcSource(this, dtg)

```
call SBroad('ChargedPtcSrcRealRate', ...)  
call SBroad('ChargedPtcSrcMcRate', ...)  
...  
call List_increment(...)  
call ChargedPtcSourceCreate(...)
```

ChargedPtcTransport(this, dtg)

```
cpt_timestep = ...  
substeps = ...
```

```
do j = 1, substeps  
  call SBroad('ChargedPtcTransportStep', ...)  
enddo
```

```
call ChargedPtcTransportStats(...)  
call ChargedPtcEnergyDep(...)
```

Usage

Usage

```
mk /global/mesh/particle/charged_ptcls
mk +source/position/...
mk +source/direction/...
mk +source/energy/...
mk +source/zaid/...
mk +source/charge/...
mk +source/mass/...
mk +source/real_rate
mk +source/mc_rate
mk +transport/...
```

```
charged_ptcls
source
position
direction
energy
zaid
charge
mass
real_rate
mc_rate
transport
```

Test Problems

Test Problems

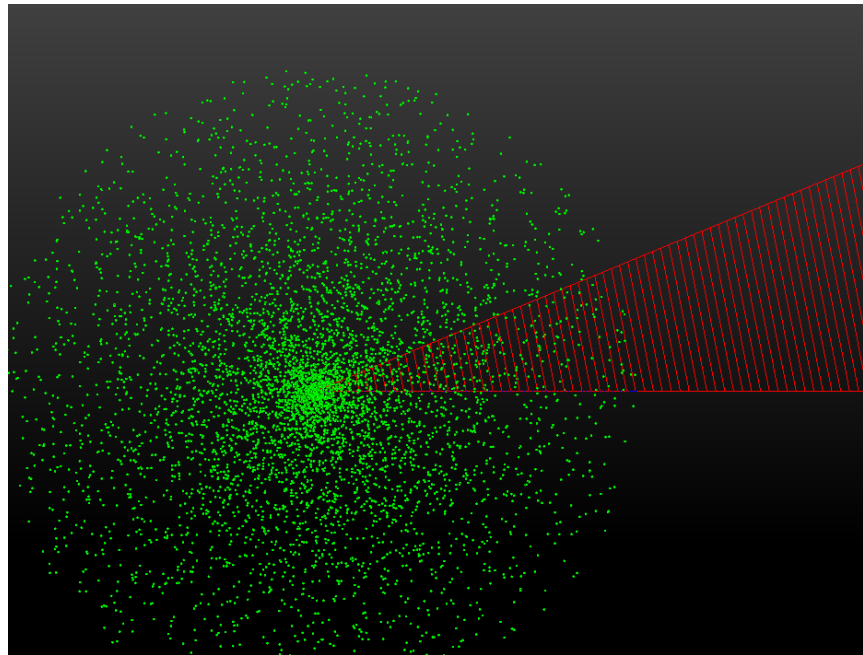
Problem #1

1D Spherical

Isotropic point source

Exercises particle tracking

No physics



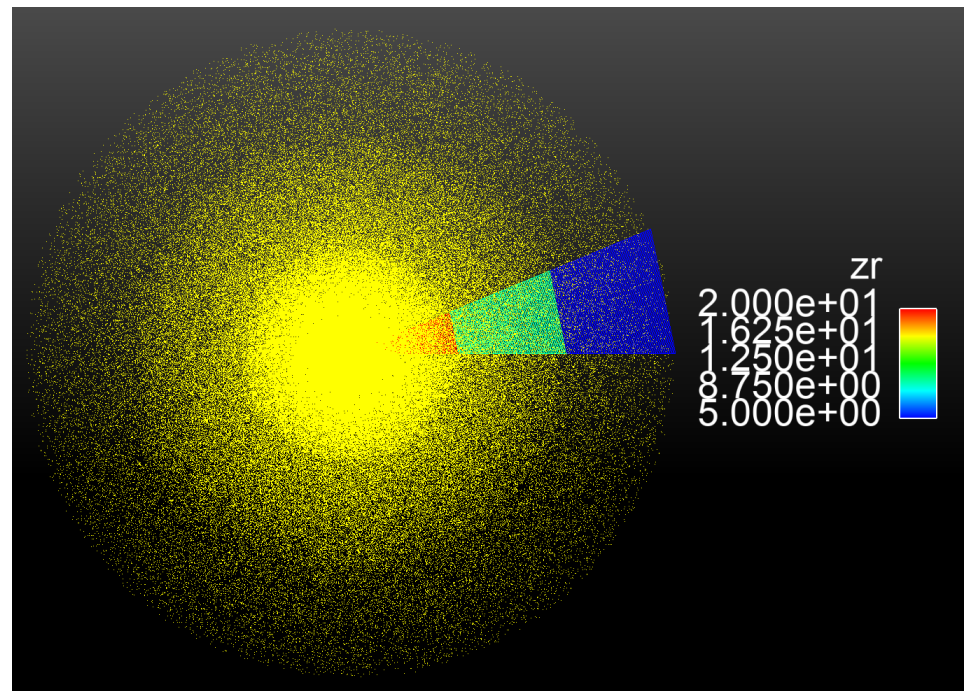
Test Problems

Problem #2

1D Spherical

Zonal source (weighted by zone density)

Simple transport



Test Problems

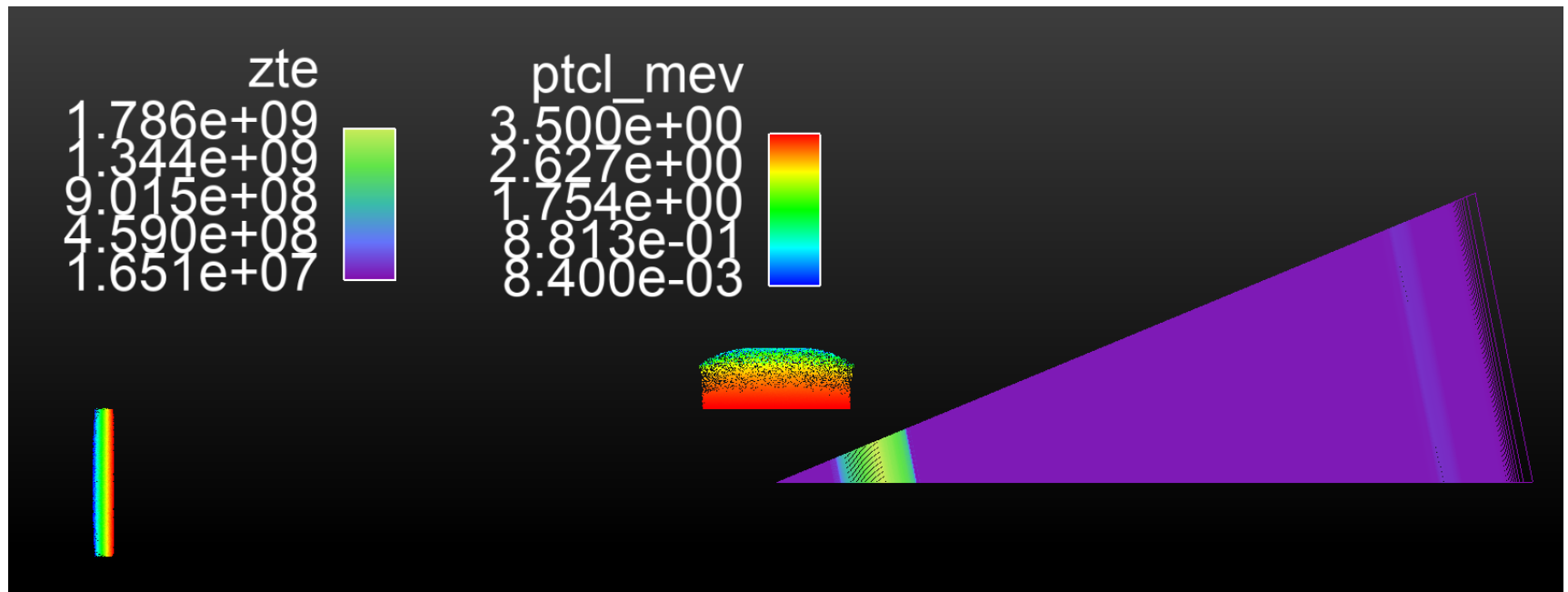
Problem #3

1D Spherical

Two mono-directional disk sources (1 particle node)

Energy coupling to matter

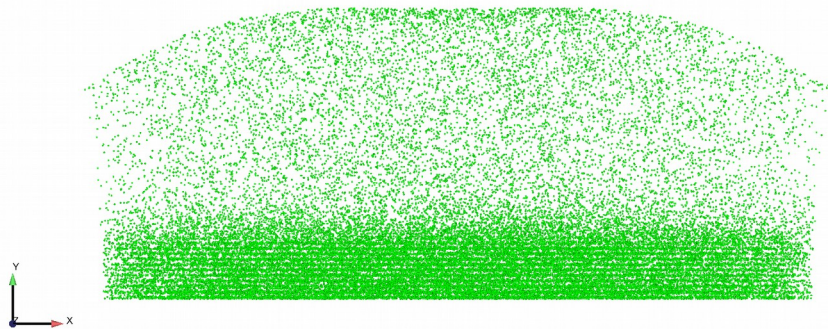
Exercises ALE+Hydro



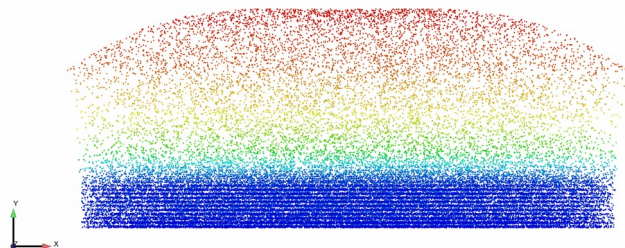
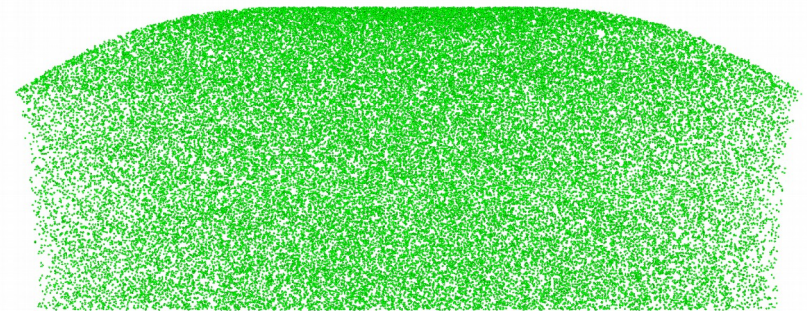
Test Problems

Problem #3

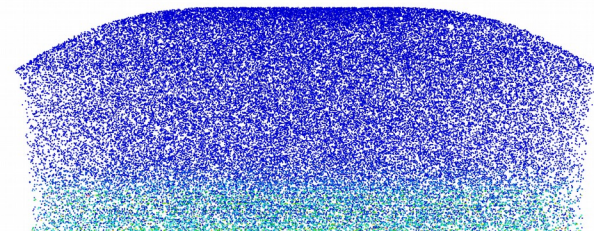
50 Particles Per Cycle



$5 < \text{Particles Per Cycle} < 500$
Weight preference = $3.5E16$



ptcr_weight
2.306e+17
1.740e+17
1.175e+17
6.104e+16
4.531e+15



ptcl_weight
4.083e+16
3.907e+16
3.792e+16
3.616e+16
3.500e+16



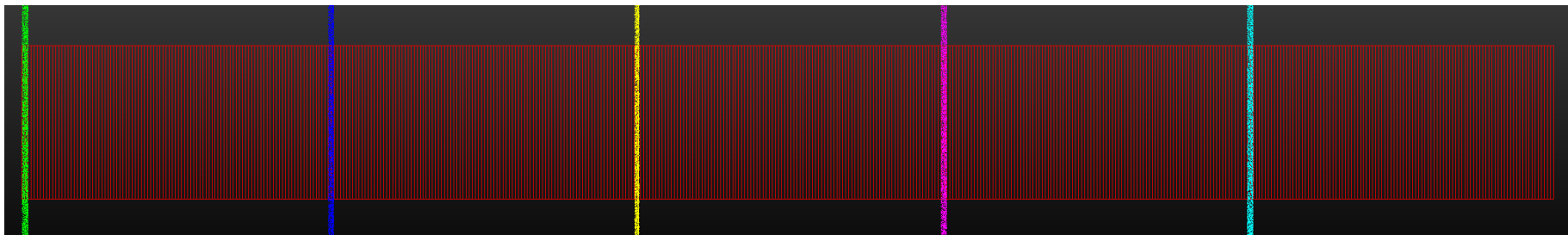
Test Problems

Problem #4

1D Cartesian

Five mono-directional disk sources (5 particle nodes)

Apple-to-apple comparison of transport methods



Simple

Simple

Analytic

Analytic

dE/dx Data

ptcl_mev1
3.495e+00
2.621e+00
1.748e+00
8.738e-01
0.000e+00



ptcl_mev2
3.494e+00
2.621e+00
1.747e+00
8.736e-01
0.000e+00



ptcl_mev3
3.491e+00
2.618e+00
1.746e+00
8.728e-01
0.000e+00



ptcl_mev4
3.496e+00
2.622e+00
1.748e+00
8.739e-01
0.000e+00



ptcl_mev5
3.496e+00
2.622e+00
1.748e+00
8.740e-01
0.000e+00



Test Problems


Problem #4

1D Cartesian


Five mono-directional disk sources (5 particle nodes)

Apple-to-apple comparison of transport methods


ptcl_mev1
3.495e+00
2.621e+00
1.748e+00
8.738e-01
0.000e+00



ptcl_mev2
3.494e+00
2.621e+00
1.747e+00
8.736e-01
0.000e+00



ptcl_mev3
3.491e+00
2.618e+00
1.746e+00
8.728e-01
0.000e+00



ptcl_mev4
3.496e+00
2.622e+00
1.748e+00
8.739e-01
0.000e+00



ptcl_mev5
3.496e+00
2.622e+00
1.748e+00
8.740e-01
0.000e+00



Simple

Simple
+
Ion Correction

Analytic
Approx.
dv/dt

Analytic
Exact
dE/dt

dE/dx Data

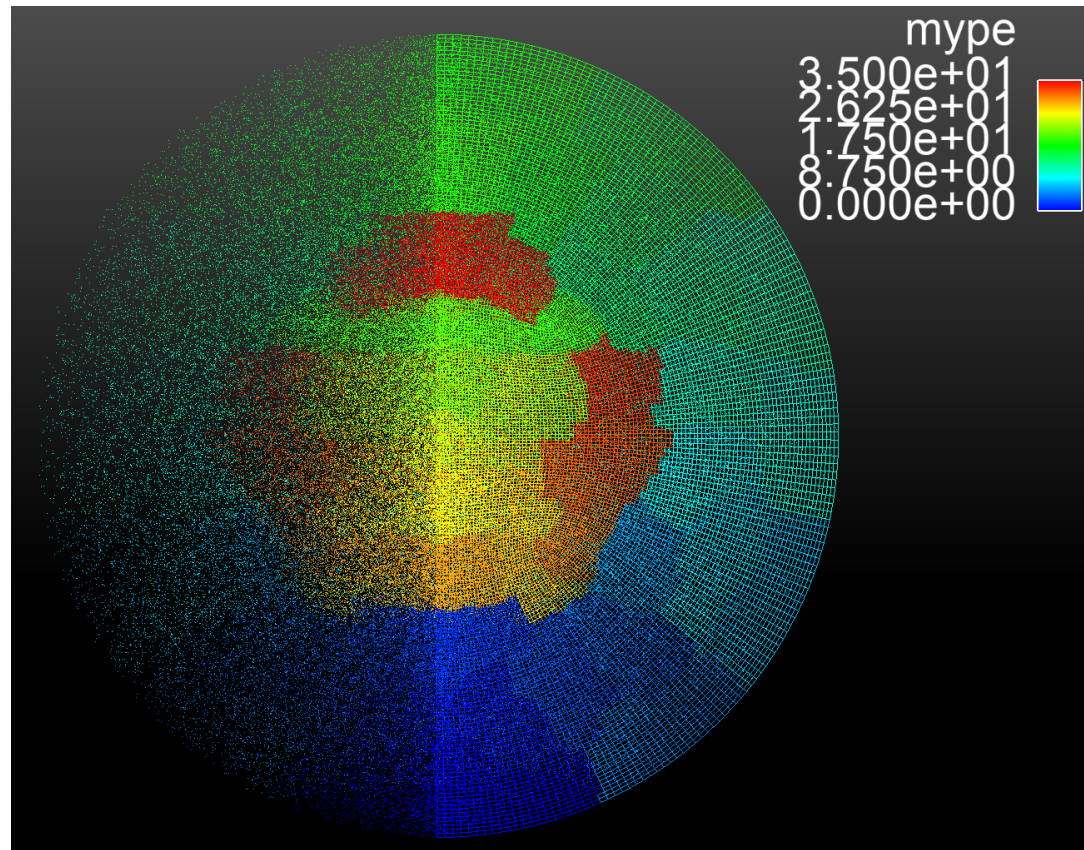
Test Problems

Problem #5

2D Cylindrical

Zonal distribution in DT

36 cores on 1 node



Future Work

Future Work

- More 2D tests
- 3D tests
- Quantitative comparison between transport methods